

chain nodes :

7 8 9 18 42 43 44 45 46 47 48 49 50 51 52 55

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 21 22 23 24 25 26 27 28 29 30 31 32  
33 34 35 36 37 38 39 40 41

chain bonds :

5-7 7-8 7-9 9-18 11-18 14-22 27-42 29-44 34-46 37-43 39-48 44-45 46-47 48-49  
50-51 51-52

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 21-22 21-26  
22-23 23-24 24-25 25-26 27-28 27-31 28-29 29-30 30-31 32-33 32-36 33-34 34-35  
35-36 37-38 37-41 38-39 39-40 40-41

exact/norm bonds :

7-8 7-9 9-18 10-11 10-15 11-12 11-18 12-13 13-14 14-15 14-22 27-28 27-31  
27-42 28-29 29-30 30-31 32-33 32-36 33-34 34-35 35-36 37-38 37-41 37-43 38-39  
39-40 39-48 40-41 44-45 46-47 48-49 50-51 51-52

exact bonds :

5-7 29-44 34-46

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26

isolated ring systems :

containing 21 :

G1:[\*1],[\*2],[\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom  
 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 21:Atom 22:Atom 23:Atom 24:Atom  
 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom  
 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:CLASS 43:CLASS  
 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS 52:CLASS  
 53:CLASS 55:CLASS

09/738022

=> s l1

SAMPLE SEARCH INITIATED 14:07:56 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 0 TO 0  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 sss full

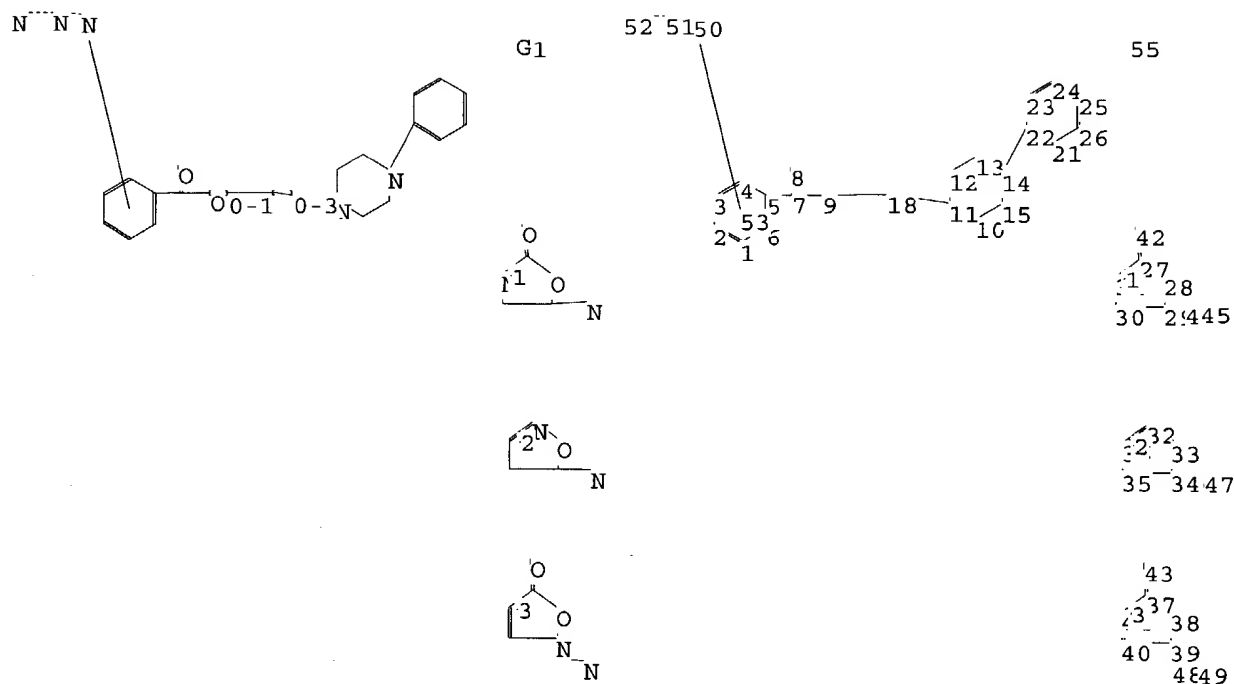
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FULL SCREEN SEARCH COMPLETED - 0 TO ITERATE

100.0% PROCESSED 0 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

L3 0 SEA SSS FUL L1

=>

Uploading C:\Program Files\Stnexp\Queries\09738022.str



chain nodes :

7 8 9 18 42 43 44 45 46 47 48 49 50 51 52 55

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 21 22 23 24 25 26 27 28 29 30  
31 32 33 34 35 36 37 38 39 40 41

chain bonds :

5-7 7-8 7-9 9-18 11-18 14-22 27-42 29-44 34-46 37-43 39-48 44-45 46-47  
48-49 50-51 51-52

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15 21-22  
21-26 22-23 23-24 24-25 25-26 27-28 27-31 28-29 29-30 30-31 32-33 32-36  
33-34 34-35 35-36 37-38 37-41 38-39 39-40 40-41

exact/norm bonds :

7-8 7-9 9-18 10-11 10-15 11-12 11-18 12-13 13-14 14-15 14-22 27-28  
27-31 27-42 28-29 29-30 30-31 32-33 32-36 33-34 34-35 35-36 37-38 37-41  
37-43 38-39 39-40 39-48 40-41 44-45 46-47 48-49 50-51 51-52

exact bonds :

09/738022

5-7 29-44 34-46

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 21-22 21-26 22-23 23-24 24-25 25-26

isolated ring systems :

containing 21 :

G1:[\*1],[\*2],[\*3]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 18:CLASS 21:Atom 22:Atom 23:Atom  
24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom  
33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom  
42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS  
50:CLASS 51:CLASS 52:CLASS 53:CLASS 55:CLASS

L4 STRUCTURE UPLOADED

=> s 14

SAMPLE SEARCH INITIATED 14:14:21 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 2 TO ITERATE

100.0% PROCESSED 2 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 2 TO 124

PROJECTED ANSWERS: 2 TO 124

L5 2 SEA SSS SAM L4

=> s 14 sss full

FULL SEARCH INITIATED 14:14:30 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 17 TO ITERATE

100.0% PROCESSED 17 ITERATIONS

10 ANSWERS

SEARCH TIME: 00.00.01

L6 10 SEA SSS FUL L4

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

315.04

315.46

FILE 'CAPLUS' ENTERED AT 14:14:35 ON 14 JUN 2004

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09/738022

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FILE COVERS 1907 - 14 Jun 2004 VOL 140 ISS 25  
FILE LAST UPDATED: 13 Jun 2004 (20040613/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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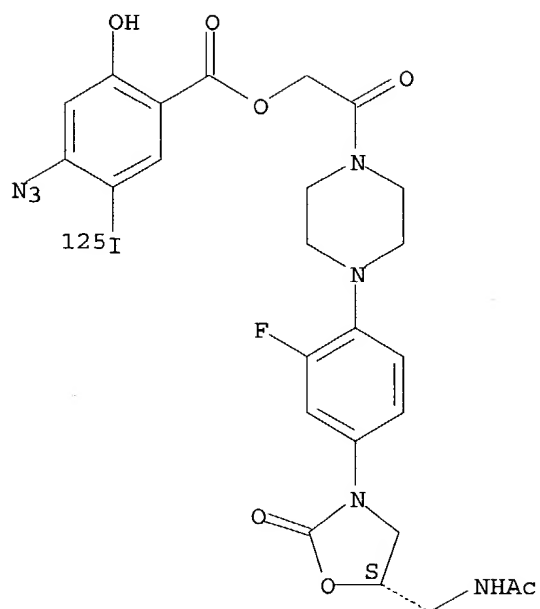
L7                    3 L6

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L7 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2003:443562 CAPLUS  
DN 139:242801  
TI Cross-linking in the Living Cell Locates the Site of Action of  
Oxazolidinone Antibiotics  
AU Colca, Jerry R.; McDonald, William G.; Waldon, Daniel J.; Thomasco, Lisa  
M.; Gadwood, Robert C.; Lund, Eric T.; Cavey, Gregory S.; Mathews, W.  
Rodney; Adams, Lonnie D.; Cecil, Eric T.; Pearson, James D.; Bock, Jeffrey  
H.; Mott, John E.; Shinabarger, Dean L.; Xiong, Liqun; Mankin, Alexander  
S.  
CS Pharmacia Corp., Kalamazoo, MI, 49001, USA  
SO Journal of Biological Chemistry (2003), 278(24), 21972-21979  
CODEN: JBCHA3; ISSN: 0021-9258  
PB American Society for Biochemistry and Molecular Biology  
DT Journal  
LA English  
AB Oxazolidinone antibiotics, an important new class of synthetic  
antibacterials, inhibit protein synthesis by interfering with ribosomal  
function. The exact site and mechanism of oxazolidinone action has not  
been elucidated. Although genetic data pointed to the ribosomal  
peptidyltransferase as the primary site of drug action, some biochem.  
studies conducted in vitro suggested interaction with different regions of  
the ribosome. These inconsistent observations obtained in vivo and in  
vitro have complicated the understanding of oxazolidinone action. To  
localize the site of oxazolidinone action in the living cell, we have  
cross-linked a photoactive drug analog to its target in intact, actively  
growing Staphylococcus aureus. The oxazolidinone cross-linked  
specifically to 23 S rRNA, tRNA, and two polypeptides. The site of  
crosslinking to 23 S rRNA was mapped to the universally conserved A-2602.  
Polypeptides cross-linked were the ribosomal protein L27, whose N terminus  
may reach the peptidyltransferase center, and LepA, a protein homologous  
to translation factors. Only ribosome-associated LepA, but not free protein,  
was cross-linked, indicating that LepA was cross-linked by the  
ribosome-bound antibiotic. The evidence suggests that a specific  
oxazolidinone binding site is formed in the translating ribosome in the  
immediate vicinity of the peptidyltransferase center.  
IT 437717-86-7, PNU 259621  
RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(site of action of oxazolidinone antibiotics in Staphylococcus aureus)  
RN 437717-86-7 CAPLUS  
CN Benzoic acid, 4-azido-2-hydroxy-5-(iodo-125I)-, 2-[4-[4-[(5S)-5-  
[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-  
2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

09/738022



RE.CNT 59      THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD  
ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/738022

L7 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

AN 2002:539929 CAPLUS

DN 137:106476

TI Oxazolidinone photoaffinity probes, uses and compounds

IN Colca, Jerry R.; McDonald, William Gerald; Shinabarger, Dean L.

PA Pharmacia & Upjohn Company, USA

SO PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DT Patent

LA English

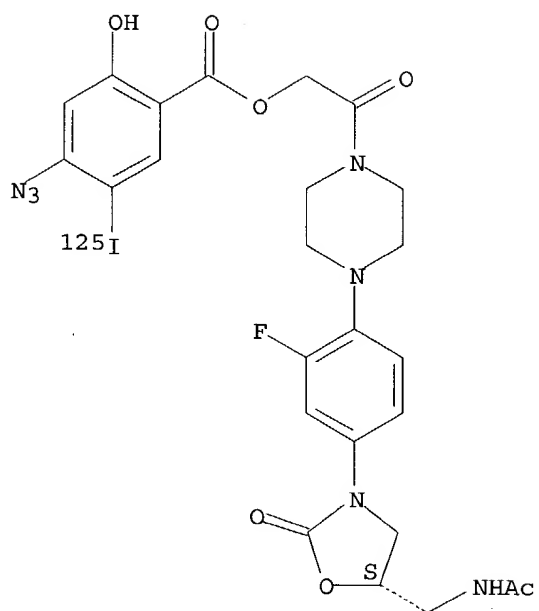
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PI	WO 2002056013	A2	20020718	WO 2001-US48455	20011214
	WO 2002056013	A3	20031106		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	EP 1386153	A2	20040204	EP 2001-993282	20011214
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
PRAI	US 2000-256053P	P	<u>20001215</u>		
	WO 2001-US48455	W	20011214		
OS	MARPAT 137:106476				
AB	Disclosed are novel methods of identifying biol. targets of compds. that have antimicrobial activity. Also disclosed are novel methods of identifying compds. that can have antimicrobial activity.				
IT	437717-86-7P 437717-87-8P 437717-88-9P 437717-89-0P				
	RL: BSU (Biological study, unclassified); IMF (Industrial manufacture); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (oxazolidinone photoaffinity probes, uses and compds.)				
RN	437717-86-7 CAPLUS				
CN	Benzoic acid, 4-azido-2-hydroxy-5-(iodo-125I)-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)				

Absolute stereochemistry.



09/738022

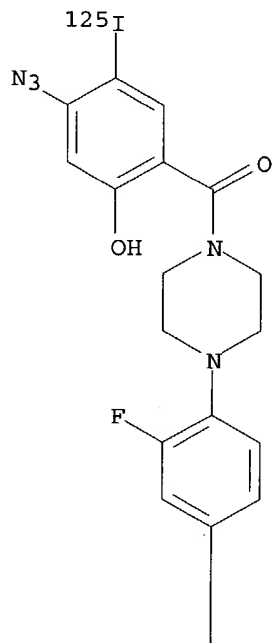


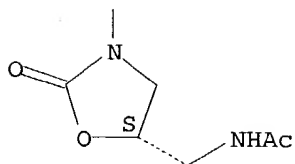
RN 437717-87-8 CAPLUS

CN Acetamide, N-[[[(5S)-3-[4-[4-[4-azido-2-hydroxy-5-(iodo-125I)benzoyl]-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

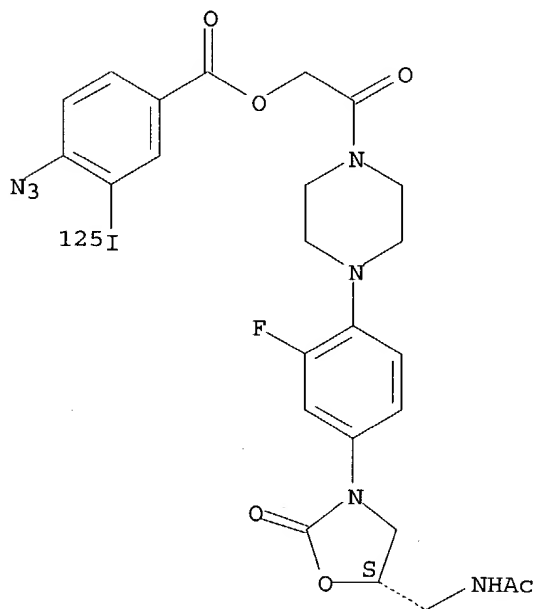




RN 437717-88-9 CAPLUS

CN Benzoic acid, 4-azido-3-(iodo-125I)-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

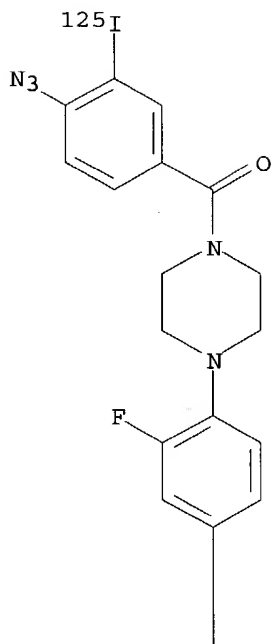


RN 437717-89-0 CAPLUS

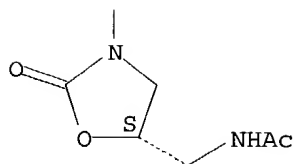
CN Acetamide, N-[[[(5S)-3-[4-[4-[4-azido-3-(iodo-125I)benzoyl]-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



IT 437717-97-0P 437717-98-1P 437717-99-2P

437718-00-8P 437718-01-9P 437718-02-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

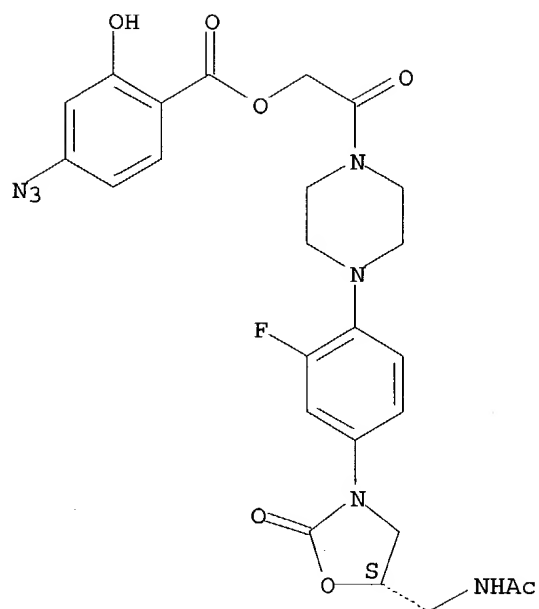
(oxazolidinone photoaffinity probes, uses and compds.)

RN 437717-97-0 CAPLUS

CN Benzoic acid, 4-azido-2-hydroxy-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

09/738022

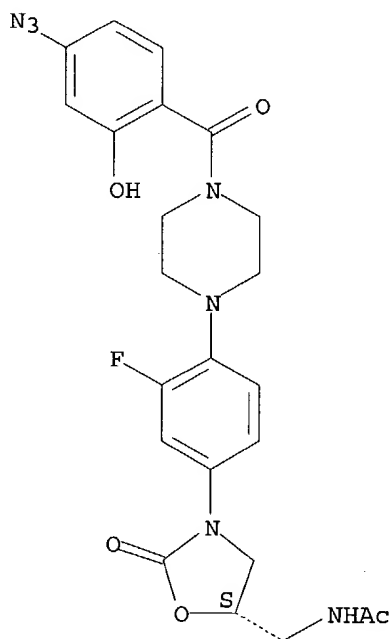


RN 437717-98-1 CAPLUS

CN Acetamide, N-[[[(5S)-3-[4-[4-(4-azido-2-hydroxybenzoyl)-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



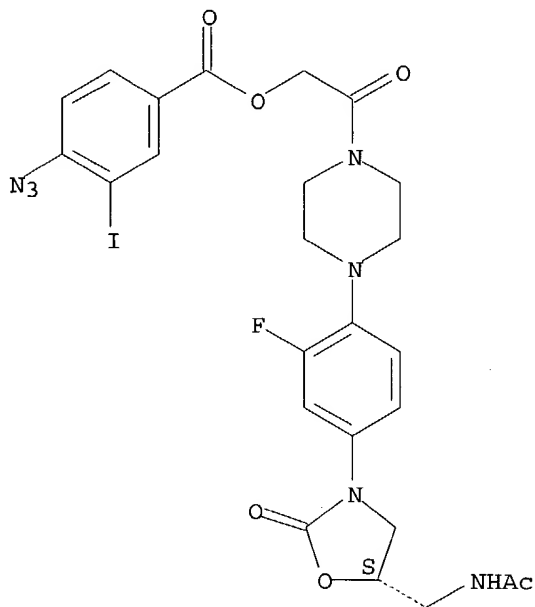
PAGE 2-A

09/738022

RN 437717-99-2 CAPLUS

CN Benzoic acid, 4-azido-3-iodo-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

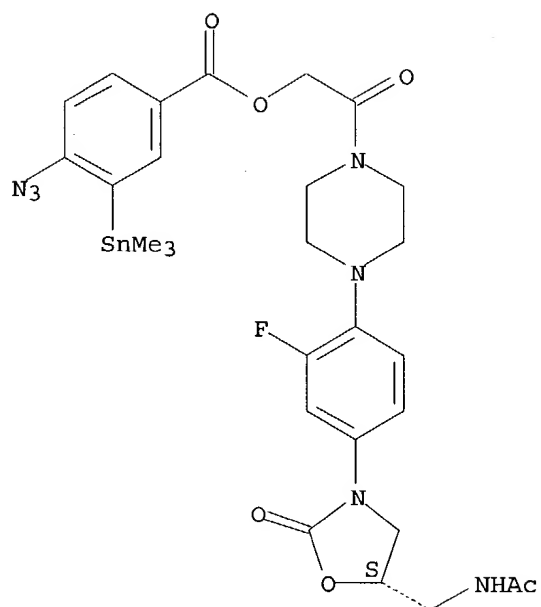


RN 437718-00-8 CAPLUS

CN Benzoic acid, 4-azido-3-(trimethylstannyl)-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

09/738022

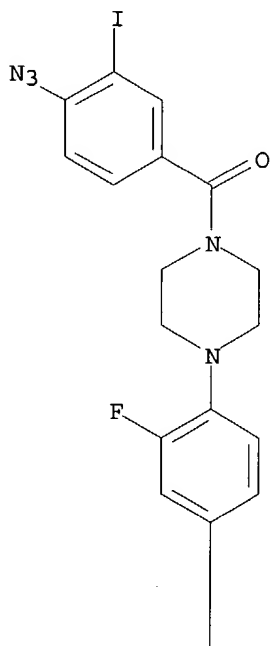


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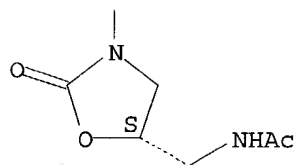
CN Acetamide, N-[[[(5S)-3-[4-[4-(4-azido-3-iodobenzoyl)-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



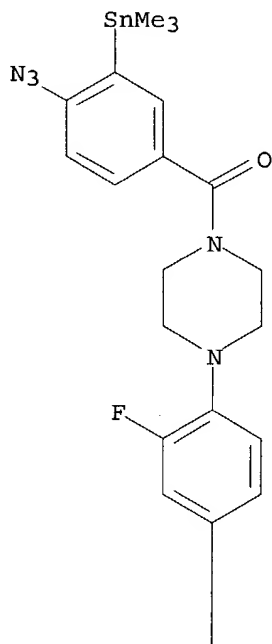
PAGE 2-A



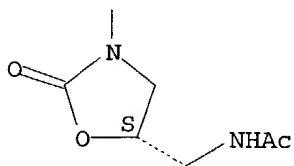
RN 437718-02-0 CAPLUS  
 CN Acetamide, N-[[ (5S)-3-[4-[4-[4-azido-3-(trimethylstannyl)benzoyl]-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A



09/738022

L7 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN  
AN 2002:465999 CAPLUS  
DN 137:33287  
TI Preparation of oxazolidinone photoaffinity probes  
IN Thomasco, Lisa Marie; Gadwood, Robert C.  
PA Pharmacia & Upjohn Company, USA  
SO PCT Int. Appl., 41 pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

APPS

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002048139	A2	20020620	WO 2001-US48063	20011214
	WO 2002048139	A3	20031002		
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	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2003073696	A1	20030417	US 2000-738022	20001215
	AU 2002034016	A5	20020624	AU 2002-34016	20011214
	EP 1368326	A2	20031210	EP 2001-985023	20011214
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
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	US 2003232008	A1	20031218	US 2003-359767	20030206
PRAI	US 2000-738022	A	20001215		
	WO 2001-US48063	W	20011214		
OS	MARPAT 137:33287				
GI					

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Title compds. I [X, Y = F, H, CH<sub>3</sub>; R<sub>1</sub> = H, F, I; R<sub>2</sub> = H, F, OH; R<sub>16</sub> = H, F; R<sub>17</sub> = H, F; R<sub>3</sub> = H, alkyl; L = bond, OCH<sub>2</sub>C(O); Q = e.g., II; R<sub>4</sub> = H, CH<sub>3</sub>, CH<sub>2</sub>CH<sub>3</sub>, cyclopropyl; Z = O, S and related analogs] were prepared For instance, (S)-N-[[3-[3-fluoro-4-[4-(hydroxyacetyl)-1-piperazinyl]phenyl]-2-oxo-5-oxazolidinyl]methyl]acetamide was coupled to 4-azidosalicylic acid (DMF, EDCI, DMAP). This intermediate was reacted with chloramine-T/NaOH/125I<sub>2</sub> to afford III. I are useful as photoaffinity probes.

IT 437717-97-0P 437717-98-1P 437717-99-2P  
437718-00-8P 437718-01-9P 437718-02-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(intermediate; preparation of oxazolidinone photoaffinity probes)

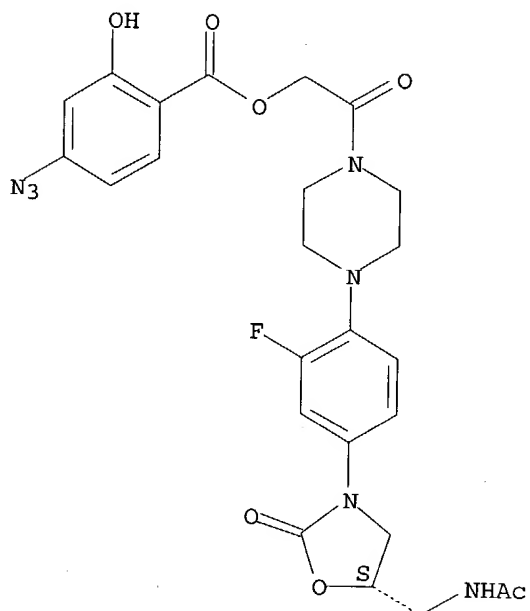
RN 437717-97-0 CAPLUS

CN Benzoic acid, 4-azido-2-hydroxy-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI)  
(CA INDEX NAME)



09/738022

Absolute stereochemistry.

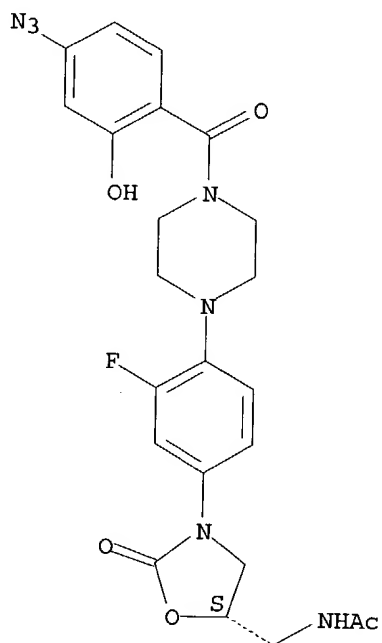


RN 437717-98-1 CAPLUS

CN Acetamide, N-[[[(5S)-3-[4-[4-(4-azido-2-hydroxybenzoyl)-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

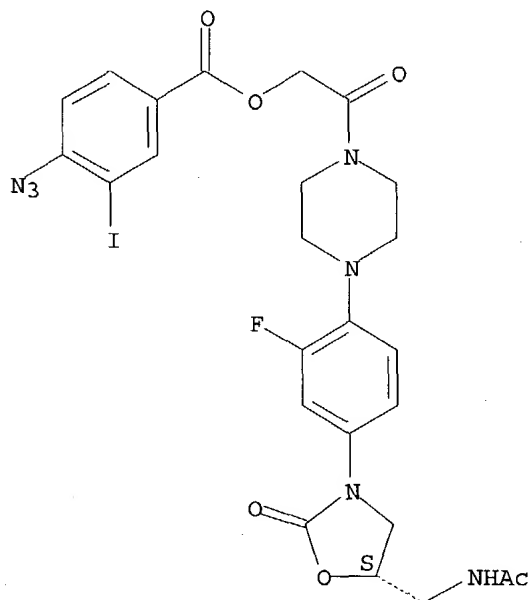
PAGE 1-A



RN 437717-99-2 CAPLUS

CN Benzoic acid, 4-azido-3-iodo-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

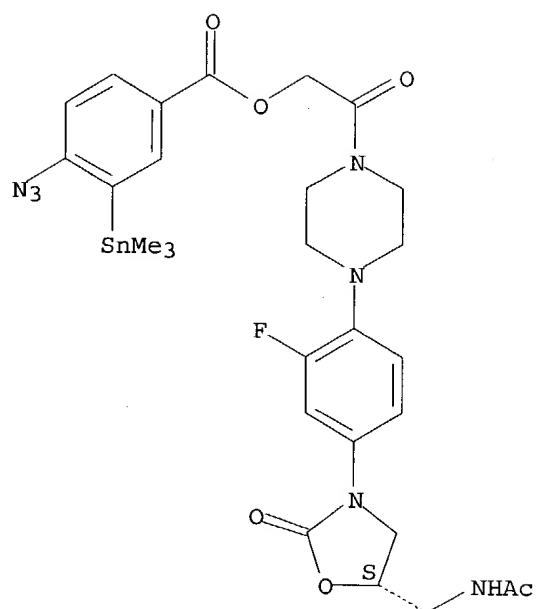


RN 437718-00-8 CAPLUS

CN Benzoic acid, 4-azido-3-(trimethylstannyl)-, 2-[4-[4-[(5S)-5-[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

09/738022

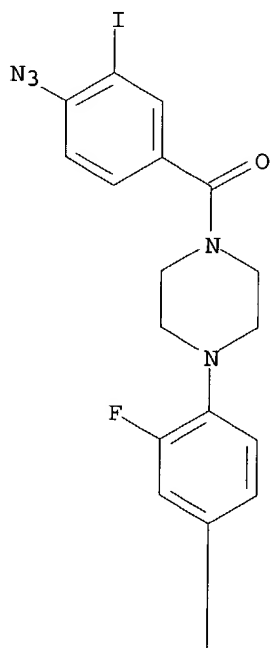


RN 437718-01-9 CAPLUS

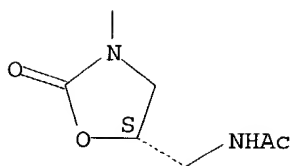
CN Acetamide, N-[[[(5S)-3-[4-[4-(4-azido-3-iodobenzoyl)-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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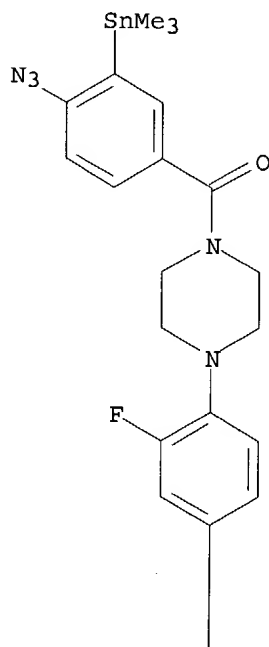
PAGE 2-A



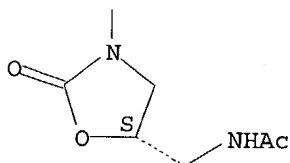
RN 437718-02-0 CAPLUS  
 CN Acetamide, N-[[[(5S)-3-[4-[4-[4-azido-3-(trimethylstannyl)benzoyl]-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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IT 437717-86-7P 437717-87-8P 437717-88-9P  
 437717-89-0P  
 RL: ANT (Analyte); BSU (Biological study, unclassified); PRP (Properties);  
 SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological

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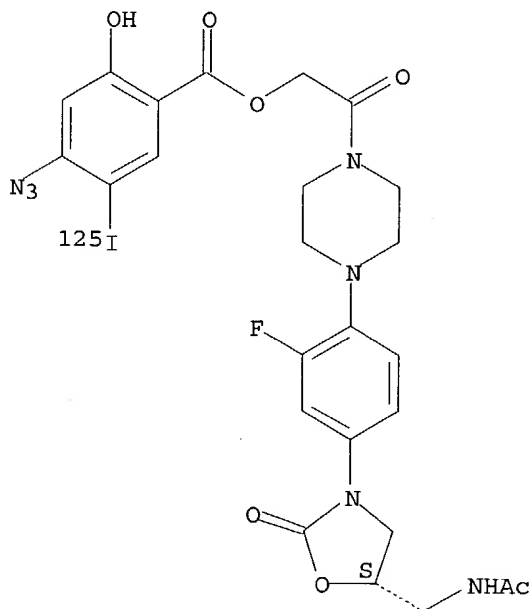
study); PREP (Preparation)

(photoaffinity probe; preparation of oxazolidinone photoaffinity probes)

RN 437717-86-7 CAPLUS

CN Benzoic acid, 4-azido-2-hydroxy-5-(iodo-125I)-, 2-[4-[4-[(5S)-5-  
[(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-  
2-oxoethyl ester (9CI) (CA INDEX NAME)

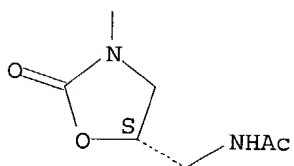
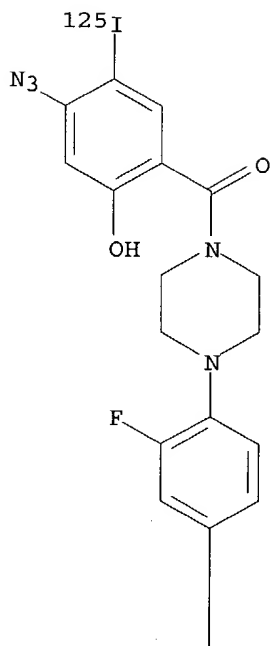
Absolute stereochemistry.



RN 437717-87-8 CAPLUS

CN Acetamide, N-[[[(5S)-3-[4-[4-[4-azido-2-hydroxy-5-(iodo-125I)benzoyl]-1-  
piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA  
INDEX NAME)

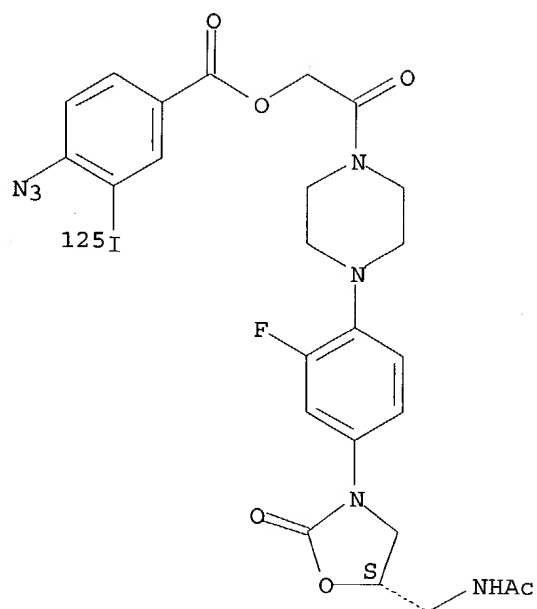
Absolute stereochemistry.



RN 437717-88-9 CAPLUS  
 CN Benzoic acid, 4-azido-3-(iodo-125I)-, 2-[4-[4-[(5S)-5-  
 [(acetylamino)methyl]-2-oxo-3-oxazolidinyl]-2-fluorophenyl]-1-piperazinyl]-  
 2-oxoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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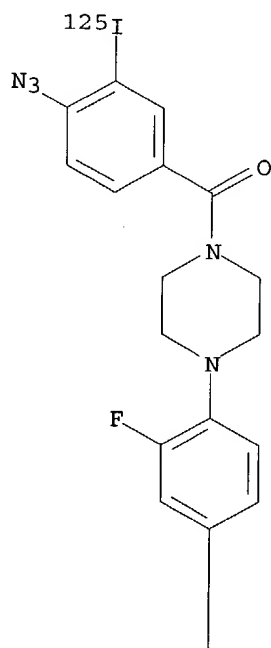


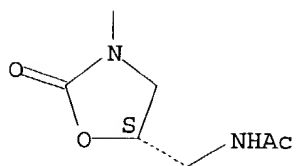
RN 437717-89-0 CAPLUS

CN Acetamide, N-[[[(5S)-3-[4-[4-azido-3-(iodo-125I)benzoyl]-1-piperazinyl]-3-fluorophenyl]-2-oxo-5-oxazolidinyl]methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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